

Competing Superconducting States in Strong Ferromagnets

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We report results from a systematic study of the competition of exotic triplet pair density wave (PDW) superconductivity (SC) with homogeneous (zero pair momentum) SC in strongly polarized media such as half metallic systems. From the two different PDW states allowed by symmetry in this background only one may dominate or even coexist with homogeneous SC. We propose a direct experimental identification of PDW SC in this context. Our results suggest that these exotic states may plausibly emerge in heterostructures involving proximity of SC with half-metallic CrO_2 where induced SC is established in the half metallic region and in strongly ferromagnetic superconductors.

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The combination of ferromagnetism and superconductivity (SC) has been a fascinating challenge for decades [1, 2] since these states are expected to compete strongly. The discovery of SC in the strongly ferromagnetic background of UGe_2 [3] has revolutionized many of our ideas on the subject opening widely the field. Additional FM superconductors have been discovered [4, 5] throwing up challenging problems such as reentrant SC [6] etc. Equally challenging are the findings in heterostructures where proximity of SC and FM is enforced [7–9]. Indeed Kaizer *et al.* reported a long distance supercurrent through the half metallic ferromagnet CrO_2 in contact with superconducting NbTiN [7]. Clearly, the proximity effect imposes bulk SC in CrO_2 despite its half metallic (fully magnetically polarized) character.

Understanding the type of exotic SC states that emerge in such extreme ferromagnetic conditions is a challenge of great theoretical and practical importance. Note that graphene nanoribbons are shown to be half metallic as well [10] opening new avenues for the nanoengineering of such states. It is natural to expect that at least in half metals SC is in the triplet channel where spins are parallel instead of being antiparallel as in usual singlet SC. Up to now, only triplet SC states with zero pair momentum have been considered in this context [11–15]. In the present Letter we argue that a different type of triplet SC states, in which the pairs have finite momentum, may dominate in the half metallic regions. These exotic SC states exhibit a density wave modulation of the superfluid density and we call them the triplet pair density wave (PDW) states or more formally the Π -triplet states.

The first studies of PDW SC in the singlet channel, also called η -pairing, were motivated by its possible realization in the pseudogap regime of cuprates [16]. Recently, experiments in the stripe-ordered materials $\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4$ and $\text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4$ [17] renewed the interest for such states [18]. A PDW state in the triplet channel as the one considered here has been suggested to occur in the high field SC state of CeCoIn_5 coexisting with singlet SC and spin density waves [19] explaining NMR [20] and fascinating neutron scattering

results [21]. This state has also been considered in the same context by Sigrist and co-workers [22]. Moreover PDW states have been suggested in the context of models for trapped fermionic gases [23].

We have examined systematically all the possible SC condensates that may emerge in a fully polarized medium and their competition within a microscopic mean field approach. The Ginzburg-Landau theory for single-spin zero pair momentum SC has been done previously [24]. Our starting point is a mean field BCS-type Hamiltonian:

$$\mathcal{H} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} - \sum_{\mathbf{k}} (\Delta_{\mathbf{k}}^0 c_{\mathbf{k}}^{\dagger} c_{-\mathbf{k}}^{\dagger} + \text{h.c.}) - \sum_{\mathbf{k}} (\Pi_{\mathbf{k}}^{\mathbf{Q}} c_{\mathbf{k}}^{\dagger} c_{-(\mathbf{k}+\mathbf{Q})}^{\dagger} + \text{h.c.}) \quad (1)$$

The Hamiltonian (1) includes no spin since we assume that we are in a strong ferromagnetic background thus all spins are frozen in the same direction. The first term describes a tetragonal tight binding dispersion which generically can be written as a sum of particle-hole symmetric terms and particle-hole asymmetric terms: $\xi_{\mathbf{k}} = \gamma_{\mathbf{k}} + \delta_{\mathbf{k}}$. When $\delta_{\mathbf{k}} = 0$ there is particle-hole symmetry or perfect nesting with the *commensurate* wavevector \mathbf{Q} while finite values of $\delta_{\mathbf{k}}$ destroy the nesting conditions. The choice of a tetragonal dispersion is motivated by the fact that CrO_2 as well as strongly FM superconductors like UGe_2 and URhGe exhibit all a tetragonal structure.

The second term $\Delta_{\mathbf{k}}^0 = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^0 \langle c_{-\mathbf{k}'} c_{\mathbf{k}'} \rangle$ represents unconventional SC with zero pair momentum, and the last term $\Pi_{\mathbf{k}}^{\mathbf{Q}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^{\mathbf{Q}} \langle c_{-(\mathbf{k}'+\mathbf{Q})} c_{\mathbf{k}'} \rangle$ unconventional SC with finite pair momentum (PDW). The effective interactions of the itinerant quasiparticles $V_{\mathbf{k},\mathbf{k}'}^0, V_{\mathbf{k},\mathbf{k}'}^{\mathbf{Q}}$ may have a purely electronic origin in the case of FM superconductors. In the case of heterostructures we assume within our approach that the effective potentials incorporate the proximity effect as well. Naturally, we would expect in that case a real space dependence of the potentials, that we neglect here. We only focus on qualitative symmetry questions that would not be affected by a smooth space dependence. Indeed the modulation of the superfluid density in our PDW SC state has a wave-

length negligible compared to the coherence length or the characteristic lengths of the heterostructure.

To treat both SC order parameters (OPs) in a compact manner we introduce a Nambu-type representation using the spinors $\Psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}}^\dagger, c_{-\mathbf{k}}, c_{\mathbf{k}+\mathbf{Q}}^\dagger, c_{-\mathbf{k}-\mathbf{Q}})$. Accordingly for the Nambu representation of the Hamiltonian in Eq. (1) we use the tensor products $\hat{\rho}_i = (\hat{\sigma}_i \otimes \hat{1}_2)$ and $\hat{\sigma}_i = (\hat{1}_2 \otimes \hat{\sigma}_i)$, where $\hat{\sigma}_i$ with $i = 1, 2, 3$ are the usual 2x2 Pauli matrices and $\hat{1}_2$ the unit 2x2 matrix. We classify the OPs with respect to their behavior under inversion (\hat{I}) $\mathbf{k} \rightarrow -\mathbf{k}$, translation ($\hat{t}_{\mathbf{Q}}$) $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{Q}$ and time reversal (\hat{T}). Instead of the latter we may use complex conjugation (\hat{K}) which is related to time reversal via the relations $\hat{T} \equiv -\hat{K}(\Delta_{\mathbf{k}}^0)$ and $\hat{T} \equiv \hat{I}\hat{K}(\Delta_{\mathbf{k}}^{\mathbf{Q}})$. Since the spins are frozen, the $\mathbf{q} = 0$ SC pair states may only have odd parity: $\Delta_{-\mathbf{k}}^0 = -\Delta_{\mathbf{k}}^0$. Under translation we have both signs $\Delta_{\mathbf{k}+\mathbf{Q}}^0 = \pm \Delta_{\mathbf{k}}^0$ and under \hat{T} we get $\hat{T}\Delta_{\mathbf{k}}^0 = -\Delta_{\mathbf{k}}^{0*}$. PDW states may have both parities $\Pi_{-\mathbf{k}}^{\mathbf{Q}} = \pm \Pi_{\mathbf{k}}^{\mathbf{Q}}$ and both signs under translation since $\Pi_{\mathbf{k}+\mathbf{Q}}^{\mathbf{Q}} = -\Pi_{-\mathbf{k}}^{\mathbf{Q}} = \mp \Pi_{\mathbf{k}}^{\mathbf{Q}}$. Time reversal demands that $\hat{T}\Pi_{\mathbf{k}}^{\mathbf{Q}} = \Pi_{-\mathbf{k}}^{\mathbf{Q}*}$ implying the relation $\hat{T} = \hat{I}\hat{K}$ for the PDW states.

The time reversal symmetry is broken due to spin freezing. This constrains us to consider only the states that are *even in time reversal in our spinless formalism*. The above symmetry properties allow *four possible SC OPs, two with zero pair momentum ($\mathbf{q} = 0$) and two with finite pair momentum: $\Delta_{\mathbf{k}}^{0I--}$, $\Delta_{\mathbf{k}}^{0I-+}$, $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$, $\Pi_{\mathbf{k}}^{\mathbf{Q}R+-}$* . Here the first index $\mathbf{q} = 0$ or $\mathbf{q} = \mathbf{Q}$ indicates the *total momentum of the pair*, the second index R or I indicates whether the OP is real or imaginary, the third index \pm indicates parity under inversion \hat{I} and the last index denotes gap symmetry under $\hat{t}_{\mathbf{Q}}$. The symmetry properties of the OPs under inversion \hat{I} and translation $\hat{t}_{\mathbf{Q}}$ imply a specific structure in \mathbf{k} -space. Every OP $M_{\mathbf{k}}$ is written in the form $M_{\mathbf{k}} = M f_{\mathbf{k}}$ where the form factors $f_{\mathbf{k}}$ belong to different irreducible representations of the tetragonal group D_{4h} . Specifically: $\Delta_{\mathbf{k}}^{0I--} \sim \sin k_x + \sin k_y$ (s-wave), $\Delta_{\mathbf{k}}^{0I-+}, \Pi_{\mathbf{k}}^{\mathbf{Q}I-+} \sim \sin(k_x + k_y)$ (p-wave) and $\Pi_{\mathbf{k}}^{\mathbf{Q}R+-} \sim \cos k_x - \cos k_y$ (d-wave).

According to the above symmetry classification there exist four possible pairs of competing SC states with zero and finite pair momentum. Using our formalism we calculate Greens functions and self-consistent systems of gap equations for each case. The competition of $\Delta_{\mathbf{k}}^{0I--}$ with $\Pi_{\mathbf{k}}^{\mathbf{Q}R+-}$ and $\Delta_{\mathbf{k}}^{0I--}$ with $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$ obey the following system of equations:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^{\Delta} \Delta_{\mathbf{k}'} \left\{ \frac{1}{4E_+(\mathbf{k}')} \tanh\left(\frac{E_+(\mathbf{k}')}{2T}\right) + \frac{1}{4E_-(\mathbf{k}')} \tanh\left(\frac{E_-(\mathbf{k}')}{2T}\right) \right\} \quad (2)$$

$$\Pi_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^{\Pi} \Pi_{\mathbf{k}'} \left\{ \frac{A(\mathbf{k}') + \gamma_{\mathbf{k}'}}{4E_+(\mathbf{k}')A(\mathbf{k}')} \tanh\left(\frac{E_+(\mathbf{k}')}{2T}\right) + \frac{A(\mathbf{k}') - \gamma_{\mathbf{k}'}}{4E_-(\mathbf{k}')A(\mathbf{k}')} \tanh\left(\frac{E_-(\mathbf{k}')}{2T}\right) \right\} \quad (3)$$

where $A(\mathbf{k}) \equiv \sqrt{\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2}$ and the quasiparticle energies are given by:

$$E_{\pm}(\mathbf{k}) = \sqrt{\left(\sqrt{\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2} \pm \gamma_{\mathbf{k}}\right)^2 + \Delta_{\mathbf{k}}^2} \quad (4)$$

The remaining two cases, competition of $\Delta_{\mathbf{k}}^{0I-+}$ with $\Pi_{\mathbf{k}}^{\mathbf{Q}R+-}$ and $\Delta_{\mathbf{k}}^{0I-+}$ with $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$, obey the following equations:

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^{\Delta} \Delta_{\mathbf{k}'} \left\{ \frac{B(\mathbf{k}') + \Pi_{\mathbf{k}'}^2}{4E_+(\mathbf{k}')B(\mathbf{k}')} \tanh\left(\frac{E_+(\mathbf{k}')}{2T}\right) + \frac{B(\mathbf{k}') - \Pi_{\mathbf{k}'}^2}{4E_-(\mathbf{k}')B(\mathbf{k}')} \tanh\left(\frac{E_-(\mathbf{k}')}{2T}\right) \right\} \quad (5)$$

$$\Pi_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}^{\Pi} \Pi_{\mathbf{k}'} \left\{ \frac{B(\mathbf{k}') + \gamma_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}{4E_+(\mathbf{k}')B(\mathbf{k}')} \tanh\left(\frac{E_+(\mathbf{k}')}{2T}\right) + \frac{B(\mathbf{k}') - \gamma_{\mathbf{k}'}^2 - \Delta_{\mathbf{k}'}^2}{4E_-(\mathbf{k}')B(\mathbf{k}')} \tanh\left(\frac{E_-(\mathbf{k}')}{2T}\right) \right\} \quad (6)$$

where $B(\mathbf{k}) \equiv \sqrt{\gamma_{\mathbf{k}}^2(\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2) + \Delta_{\mathbf{k}}^2 \Pi_{\mathbf{k}}^2}$ and the dispersion relations take the form:

$$E_{\pm}(\mathbf{k}) = \sqrt{\frac{\Delta_{\mathbf{k}}^2 \delta_{\mathbf{k}}^2}{\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2} + \left(\sqrt{\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2} \pm \sqrt{\gamma_{\mathbf{k}}^2 + \frac{\Delta_{\mathbf{k}}^2 \Pi_{\mathbf{k}}^2}{\delta_{\mathbf{k}}^2 + \Pi_{\mathbf{k}}^2}} \right)^2} \quad (7)$$

The effective potentials $V_{\mathbf{k},\mathbf{k}'}^{\Delta}, V_{\mathbf{k},\mathbf{k}'}^{\Pi}$ have the form $V_{\mathbf{k},\mathbf{k}'} = V f_{\mathbf{k}} f_{\mathbf{k}'}$ (separable potentials). We have solved self consistently the systems of equations (2), (3) and (5), (6) on a square lattice with $\gamma_{\mathbf{k}} = -t_1(\cos k_x + \cos k_y)$ and $\delta_{\mathbf{k}} = -t_2 \cos k_x \cos k_y$ and $\mathbf{Q} = (\pi, \pi)$. For every competing pair we have performed a large number of self-consistent calculations varying the pairing potential in the two channels, the temperature and the ratio t_2/t_1 .

The first important result is that the $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$ OP can never survive when it competes with any of the two zero pair momentum SC states. Specifically, the $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$ gap is zero regardless of the values of the pairing potentials and the particle-hole asymmetry term. Therefore, *although the state $\Pi_{\mathbf{k}}^{\mathbf{Q}I-+}$ is allowed by symmetry it is never realized*. We report here

results from the competition of the remaining PDW OP $\Pi_{\mathbf{k}}^{QR+-}$ with both zero momentum SC states. The phase sequences as t_2/t_1 grows starting from zero with respect to the values of the effective potentials for the competition $\Pi_{\mathbf{k}}^{QR+-}$ with $\Delta_{\mathbf{k}}^{OI--}$ and $\Pi_{\mathbf{k}}^{QR+-}$ with $\Delta_{\mathbf{k}}^{OI+-}$ are shown in Fig. 1. Arrows in Fig. 1 indicate the cascade of phases observed when the ratio t_2/t_1 grows starting from zero. Since we consider a spin-polarized background, all states reported also coexist with FM, and the transitions to the FM state reported at high values of t_2/t_1 has the meaning of a transition to a state that is only ferromagnetic with no SC OP present.

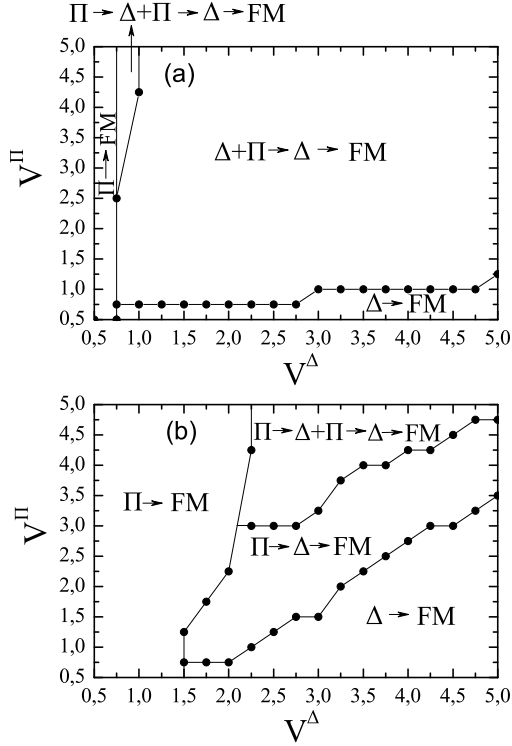


FIG. 1. Maps of the dependence of phase sequences on the effective interactions V^Δ and V^Π for low temperature. Arrows indicate the cascade of phases obtained when t_2/t_1 grows starting from zero. The black dots separate regions of different phase sequences under growing t_2/t_1 . All phases coexist with ferromagnetism (FM). The phases indicated as FM, are phases in which there is not any finite Δ or Π OP and so only FM is present. Panel (a) corresponds to the competition of $\Pi_{\mathbf{k}}^{QR+-}$ with $\Delta_{\mathbf{k}}^{OI--}$. Panel (b) corresponds to the competition of $\Pi_{\mathbf{k}}^{QR+-}$ with $\Delta_{\mathbf{k}}^{OI+-}$. The potentials are in units of t_1 .

The competition of $\Pi_{\mathbf{k}}^{QR+-}$ with $\Delta_{\mathbf{k}}^{OI--}$ favors the coexistence of both SC states ($\mathbf{q} = \mathbf{0}$ and $\mathbf{q} = \mathbf{Q}$) in low-T over a wide range of values of the pairing potentials (Fig. 1a). The transition from a coexistence state to a SC state with $\mathbf{q} = \mathbf{0}$ when t_2/t_1 grows is always continuous (second order) and dominates the V^Δ, V^Π parameter space.

The low temperature regime is different when $\Pi_{\mathbf{k}}^{QR+-}$ competes with $\Delta_{\mathbf{k}}^{OI+-}$. Coexistence of the two SC states is allowed again but is restricted only to a small portion of V^Δ, V^Π space (Fig. 1b) compared with the previous case. The most interesting feature of the V^Δ, V^Π map is the domination of the PDW state for the smaller values of t_2/t_1 . Thus, in this case the formation of the $\Pi_{\mathbf{k}}^{QR+-}$ PDW state is favored. As particle hole asymmetry grows (t_2/t_1 grows) we may have transitions from PDW to a state of coexistence or to a zero pair momentum SC state. We report in Fig. 2 the dependence of the OPs on t_2/t_1 at low-T (Fig. 2a) and the phase diagram (Fig. 2b) obtained for $V^\Delta = V^\Pi = 3$. These values correspond to the transition $\Pi \rightarrow \Delta \rightarrow FM$ of Fig. 1b. At low-T the transition from the PDW to the Δ state is first order in t_2/t_1 , and we note that the PDW gap is significantly larger than the Δ gap although the pairing potentials have the same magnitude (Fig. 2a). The phase diagram shows that the transition $\Pi \rightarrow \Delta$ with t_2/t_1 is not limited to low-T. The PDW phase extends to higher temperatures (Fig. 2b) than the Δ -phase. The boundary separating the two SC states is first order and ends at a tricritical point. Decreasing the temperature moves the boundary to lower t_2/t_1 -values. This allows a first order transition with respect to temperature within the superconducting phase from the Π to Δ state. An example of such a transition realized for $t_2/t_1 = 2$ is shown in the inset of Fig. 2b.

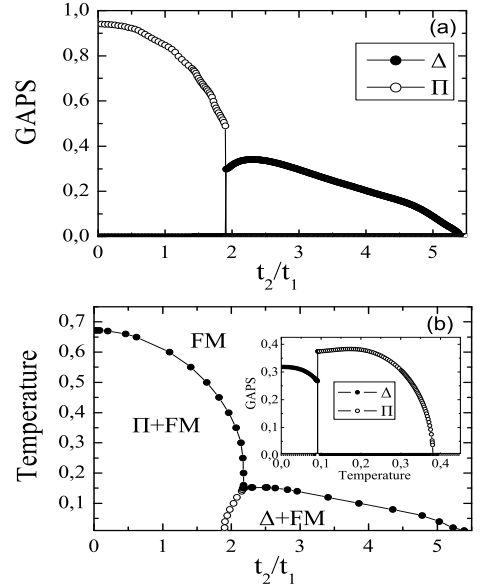


FIG. 2. (a) Dependence of $\Delta_{\mathbf{k}}^{OI+-}$ and $\Pi_{\mathbf{k}}^{QR+-}$ on t_2/t_1 in low-T. (b) t_2/t_1 -temperature phase diagram. Closed symbols mark 2nd order and open symbols 1st order transitions. A transition within the SC phase, from the PDW state to the $\Delta_{\mathbf{k}}^{OI+-}$ state, is possible with decreasing temperature. The values of the pairing potentials are $V^\Delta = V^\Pi = 3$.

A question that naturally emerges is how the exotic

PDW state $\Pi_{\mathbf{k}}^{QR+-}$ can be identified experimentally. Quite remarkably, specific heat measurements at low-T may be enough. Both SC states of zero pair momentum exhibit a polynomial behavior of the specific heat in the low temperature regime and this also the case when $\Pi_{\mathbf{k}}^{QR+-}$ coexists with either of the two SC states of zero pair momentum. On the other hand when purely $\Pi_{\mathbf{k}}^{QR+-}$ state is present the specific heat at low-T exhibits a linear temperature behavior. We illustrate that in Fig. 3 where the Fermi surface and the specific heat for $t_2/t_1 = 1.0$ in the PDW-phase (upper panel) and $t_2/t_1 = 2.5$ in the Δ -phase (lower panel) are reported. We observe that in the $\Pi_{\mathbf{k}}^{QR+-}$ phase the Fermi surface is extended imposing a linear specific heat at low-T. On the contrary, in the $\Delta_{\mathbf{k}}^{OI+-}$ phase we have only two Fermi points and the specific heat at low-T exhibits a polynomial dependence. This is also the case for the other homogeneous SC state $\Delta_{\mathbf{k}}^{OI--}$. Therefore *linear low-T specific heat identifies the PDW state*.

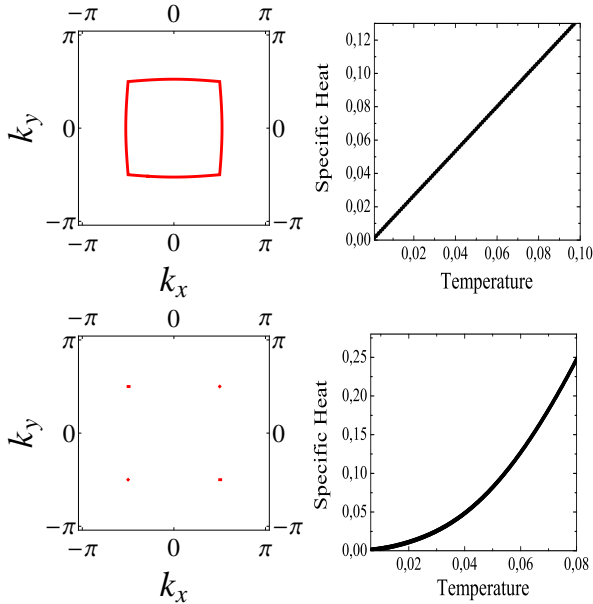


FIG. 3. Fermi surface (left) and specific heat at low-T (right) in the $\Pi_{\mathbf{k}}^{QR+-}$ phase $t_2/t_1 = 1.0$ (upper panel) and in the $\Delta_{\mathbf{k}}^{OI+-}$ phase $t_2/t_1 = 2.5$ (lower panel).

In summary, we explored systematically the possibility that exotic triplet PDW states may dominate or coexist with usual triplet SC states of zero pair momentum in a fully polarized electronic system. We find that two SC states with zero ($\mathbf{q} = \mathbf{0}$) and two SC states with finite ($\mathbf{q} = \mathbf{Q}$) pair momentum are allowed by symmetry in this context. Our calculations showed that the PDW state $\Pi_{\mathbf{k}}^{QR+-}$ having the p-wave symmetry can never survive when it competes with any of the two SC states of zero pair momentum. The other PDW $\Pi_{\mathbf{k}}^{QR+-}$ having d-wave symmetry may *either appear alone dominating upon the SC states of zero pair momentum or coexist with them*.

Specific heat measurements in low-T can identify this exotic PDW phase that may plausibly develop in Superconductor - half metal heterostructures and in strongly ferromagnetic superconductors as well.

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